Convergence to walls of dislocations in the periodic case

M. Al Haj[*], Ł. Paszkowski[†]

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Abstract

In this paper we are interested in the convergence of accumulation of dislocations to walls of dislocations. We consider the dynamical system generated by the force $f(x,y) = \frac{x(y^2-x^2)}{(y^2+x^2)^2}$, defined over $\mathbb{R} \times \mathbb{Z}\backslash\{0\}$, that describes the phenomena. For initial data $X^0 \in \Omega \cap \ell^\infty = \left\{X : |x_i - x_j| \leqslant \sqrt{3-2\sqrt{2}}\,|i-j|\right\} \cap \ell^\infty$, we show the existence of unique solution $X \in C^1 \in ([0,+\infty), \Omega \cap \ell^\infty)$. Moreover, we prove that if X^0 is periodic, then $X(t) = (x_j(t))_{j\in\mathbb{Z}}$ is periodic for any $t > 0$ and converges to the barycenter of the initial data, i.e. $x_j(t) \to c = \frac{1}{N}\sum_{i=1}^N x_i^0$ for every $j \in \mathbb{Z}$. We also establish a ℓ^p contraction for periodic solutions and perform numerical simulations.

Keywords: Dynamical system, Cauchy Lipschitz theorem, comparison principle, periodic solution, viscosity solutions.

1 Introduction

It is well known, in real materials with dislocations, that we can observe several accumulation of dislocations in walls of dislocations or more general in cells with several walls. In this paper our aim is to investigate the dynamics of dislocations that interact together and converge to such walls of dislocations.

[*]CERMICS, Ecole des Ponts ParisTech, 6 et 8 avenue Blaise Pascal, Cité Descartes Champs-sur-Marne, 77455 Marne-la-Vallée Cedex 2, France, e-mail: alhajm@cermics.enpc.fr

[†]Uniwersytet Wrocławski, pl. Grunwaldzki 2/4, 50–384 Wrocław, Poland, e-mail: lukasz.paszkowski@math.uni.wroc.pl

1.1 Presenting the problem

Let us consider a model describing horizontal motion of dislocation lines parallel to the z-axis. Considering the cross section of these lines, we can reduce the problem to its two-dimensional counterpart where each dislocation line is represented by its position $(x_i(t), i) \in \mathbb{R} \times \mathbb{Z}$. Finally, such horizontal evolution can be characterized as follows

$$x_i' = \sum_{j \neq i} f(x_j - x_i, j - i) \quad \text{for} \quad i \in \mathbb{Z}. \tag{1.1}$$

Here $f\colon \mathbb{R} \times \mathbb{Z} \backslash \{0\} \to \mathbb{R}$ is an anisotropic force of two-body interactions. An example of such a force, according to [6], is

$$f(x, y) = \frac{x(y^2 - x^2)}{(y^2 + x^2)^2}. \tag{1.2}$$

An important aspect of interatomic interactions is that atoms can attract each other at longer distances and repel at short distances aggregating into various bulk forms. Such behaviour, of course, depends on the form of the considered potentials.

One of the forces describing both long-range attraction and short-range repulsion between atoms is the interaction force given by (1.2). In such an example two particles attract each other if the vertical angle between them is less then $\frac{\pi}{4}$ and, on the other hand, repel each other if the angle is greater then $\frac{\pi}{4}$, see Figure 1 and Figure 2.

In the literature, however, there is a convention to express force in terms of energy potentials or commonly called *interatomic potentials*. Thus a general force acting on an atom can be seen as the negative derivative of some potential function with respect to its position: $f(r) = -\phi'(r)$.

The system of all particles acting together under the force defined in (1.2) can be rewritten in the following way

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} X(t) = F(X(t)), & t > 0, \\ X(0) = X^0, \end{cases} \tag{1.3}$$

where $X(t) = (x_i(t))_{i \in \mathbb{Z}}, F(X) = (F_i(X))_{i \in \mathbb{Z}}$ and X^0 is some given initial position of dislocations. Moreover, $F_i(X)$ describes a resultant force acting on an i-th particle, *i.e.*

$$F_i(X) \stackrel{def}{=} \sum_{j \neq i} f(x_j - x_i, j - i) \quad \text{for each} \quad i \in \mathbb{Z}.$$

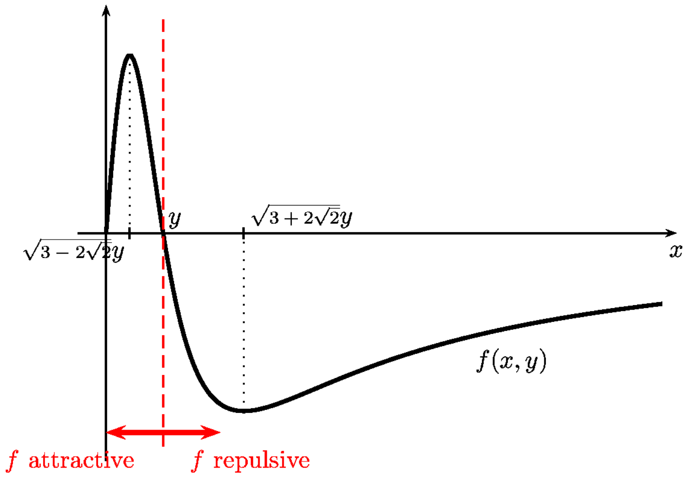

Figure 1: Interaction force $f(x, y)$ as a function of the distance between two atoms for some fixed $y \in \mathbb{Z}\backslash\{0\}$ with the property $f(-x, y) = -f(x, y)$. A vertical angle between two particles corresponds to $\arctan(\frac{x}{y})$. Thus $\frac{\pi}{4}$ reads as $x = |y|$.

Since our aim is to study a long time behaviour of the dynamics of particles which converges to walls of dislocations, the property of the force f described in (1.2) forces us to consider the problem (1.3) with a special condition for the initial data. Namely, we assume

$$f(x, y) = \frac{x(y^2 - x^2)}{(y^2 + x^2)^2}, \tag{1.4a}$$

$$X^0 \in \Omega \cap \ell^\infty, \tag{1.4b}$$

where

$$\Omega = \left\{ X : |x_i - x_j| \leqslant \sqrt{3 - 2\sqrt{2}}\,|i - j| \right\}. \tag{1.5}$$

and $\ell^\infty = \ell^\infty(\mathbb{R})$ is the Banach space of all bounded sequences over $\mathbb{R}$ supplemented with the norm $\|\cdot\|_\infty = \sup_{n\in\mathbb{Z}} |x_n|$.

Remark 1.1 (Sign of f when $X \in \Omega$)**.** *If $X(t) = (x_i(t))_{i\in\mathbb{Z}} \in \Omega$, then, in particular, we have $(j - i)^2 \geq (x_j - x_i)^2$. This implies that if $X \in \Omega$, then (because of* (1.2)*) $f(x_j - x_i, j - i)$ has the sign as $x_j - x_i$.*

Notice here that $\arctan\left(\sqrt{3 - 2\sqrt{2}}\right) = \frac{\pi}{8}$ guarantees that the force f restricted to Ω is not only attractive but also non-decreasing with respect to the first variable. Therefore, we are able to prove a comparison principle, which helps us to conclude *e.g.* existence of global-in-time solutions, which stays in Ω.

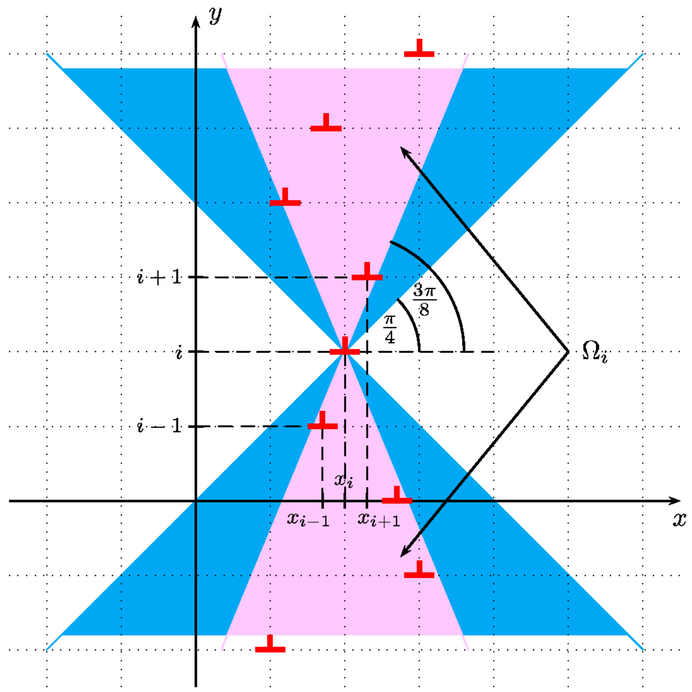

Figure 2: A fixed particle x_i attracts all other particles if they are placed in a region marked in blue and pink. However, the force f is non-decreasing only if the particles are located in the region marked in pink. Such domain we call Ω_i and thus we can present Ω, defined in (1.5), as $\Omega = \cap_{i\in\mathbb{Z}}\Omega_i$.

1.2 Main results

Our first result deals with the existence of solutions to the considered problem. More precisely, it reads as follows

Theorem 1.2 (Existence of a unique solution)**.** *Let* (1.4) *hold. Then there exists a unique solution* $X \in C^1([0,+\infty), \Omega \cap \ell^\infty)$ *of the Cauchy problem* (1.3)*. Moreover, if the initial data* X^0 *is* N*-periodic (i.e.* $x_i^0 = x_{i+N}^0$*, for every* $i \in \mathbb{Z}$*), then the solution remains* N*-periodic for every time* $t > 0$.

The proof of the theorem consists in the application of the classical Cauchy-Lipschitz theorem and the comparison principle result. Notice that in general the locally Lipschitz condition with respect to the first variable of the function f is sufficient to obtain a unique local-in-time solution. In order to extend it to the global-in-time one we need to provide an apriori estimate, *e.g.* the comparison principle that ensures us that ℓ^∞-norm of the solution does not blow up.

However, if the function f satisfies the Lipschitz condition globally, which happens when f is defined by (1.4a), we immediately obtain a unique global-in-time solution by extending it with the universal step $T > 0$, see [2, Thm 7.3, p. 184]. Thus, in that case the comparison principle is needed only to ensure that the solution belongs to Ω for all times $t > 0$.

To prove the comparison principle for the problem (1.3), the monotonicity of a function f is a necessary assumption. Hence, the reason why we consider the initial condition in the special domain Ω is that the function f defined by (1.4a) is indeed monotone over that set.

Our second result is the long time behaviour of the dynamics of particles where we prove that dislocations accumulate creating so-called walls of dislocations. This result can be stated in the following way

Theorem 1.3 (Convergence to flat walls)**.** *Let X be the N-periodic solution of the problem* (1.3)-(1.4)*. Then it converges to a constant stationary solution of the problem* (1.3)-(1.4) *i.e. for every $i \in \mathbb{Z}$, we have $\lim_{t\to\infty} x_i(t) = c$, where $c = \frac{1}{N}\sum_{i=1}^N x_i^0$ is the barycenter of the initial data.*

For the proof of the above theorem we refer to Section 4, and Section 6 for numerical experiments which show the convergence and more information.

We have also proved the following ℓ^p contraction for periodic solutions:

Proposition 1.4 (l^p contraction)**.** *Let X and Y be two N-periodic solutions of the problem* (1.3)-(1.4) *with N-periodic initial data X^0 and Y^0 respectively. Then the following estimate*

$$\|X(t) - Y(t)\|_p \leqslant \|X^0 - Y^0\|_p, \quad \textit{for all } t > 0$$

holds true provided $p \geqslant 2$.

1.3 Related results

Another possible model, first proposed in 1924 and repeatedly improved in subsequent years, involves the Lennard-Jones potential [7]

$$\phi(r) = 4\varepsilon\left[\left(\frac{r}{\sigma_0}\right)^{-12} - \left(\frac{r}{\sigma_0}\right)^{-6}\right],$$

where r is a distance between two atoms, ε is the depth (minimum) of the energy and σ_0 is the finite distance at which the interparticle potential is zero. Due to its computational simplicity and relatively good approximations, the Lennard-Jones potential is extensively used to describe the properties of gases and in computer simulations [7, 8].

There is no necessity to deal only with two-body potentials. One approach to represent the many-body potentials energy is to consider it as a sum of two-body, three-body, ..., N-body terms. An example of such constructed energy potential is the Stillinger-Weber potential [10] for semiconductor silicon containing only two- and three-body terms.

More facts about dislocations, examples of potentials used in various models, and numerical simulations performed on these models can be found in the book of Bulatov and Cai [3].

A similar model to ours, where a finite number of dislocations of different types occur (for instance positive and negative ones), was considered by El Hajj, Ibrahim and Monneau [6]. The authors studied horizontal motion of dislocation lines and they derived formally a two-dimensional mean field model called Groma-Balogh model. In the same paper, they also investigated a model with additional boundary conditions. They observed that positive dislocations move to the right, whereas the negative ones move to the left. In particular, numerical simulations of deformations of a slab under an external shear stress have been performed.

Related models called *individual cell-based* models occur not only in the theory of dislocations but also in the study of *e.g.* chemotherapy where x_i denotes a center of a tumour cell [5], chemotaxis [9] and many others. Moreover, particles may also evolve according to stochastic differential equations, see [1] and references therein for numerical simulations.

2 Comparison principle

In this section, we prove a comparison principle result for a general system of equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = G(X(t)), \quad t > 0, \tag{2.1}$$

where $X(t) = (x_i(t))_{i\in\mathbb{Z}}, G(X) = (G_i(X))_{i\in\mathbb{Z}}$ with $G_i(X) \overset{def}{=} \sum_{j\neq i} g(x_j - x_i, j-i)$ for each $i \in \mathbb{Z}$, and $g\colon \mathbb{R}\times\mathbb{Z}\backslash\{0\} \to \mathbb{R}$ is C^1 and globally non-decreasing with respect to first variable. We will apply this later in Section 3.

Lemma 2.1 (Comparison principle). *Let $T > 0$ and assume that $X, Y \in C^1([0,T), \ell^\infty)$ be two solutions of (2.1) with $X(0) = X^0$ and $Y(0) = Y^0$. Assume that $X^0 \leqslant Y^0$, then $X(t) \leqslant Y(t)$ for every $t \in [0,T)$.*

Proof. Notice that the assumption $X^0 = X(0) \leqslant Y(0) = Y^0$ reads as $x_n^0 := x_n(0) \leqslant y_n(0) =: y_n^0$ for every $n \in \mathbb{Z}$, and we shall prove that $x_n(t) \leqslant y_n(t)$ for every $n \in \mathbb{Z}$ and $t \in [0,T)$.

Define then new functions $Z(t) = (z_n(t))_{n\in\mathbb{Z}}$ and $M(t)$ as

$$z_n(t) = x_n(t) - y_n(t), \quad M(t) = \sup_{n\in\mathbb{Z}} z_n(t). \tag{2.2}$$

Since $X(t)$, $Y(t) \in \ell^\infty$ for all $t \in [0,T)$, then from the definition of M, we have

$$\forall_{t^*\in[0,T)}\, \exists_{n^*(t^*)}\ M(t^*) = z_{n^*(t^*)}(t^*), \tag{2.3}$$

where $n^*(t^*)$ may not be necessarily finite. Our goal is to show that

$$M(t) \leqslant 0 \quad \text{ for all times } t \in [0,T). \tag{2.4}$$

The way to prove (2.4) is to show that for all $t \in [0,T)$, we have $M'(t) \leq 0$ in the viscosity sense. Then by a comparison principle or the Gronwall inequality we deduce (2.4).

Step 1: $n^*(t^*) \in \mathbb{Z}$.
Let $t^* \in [0,T)$ and consider a test function ϕ such that

$$\begin{cases} M(t) \leqslant \phi(t), \\ M(t^*) = \phi(t^*). \end{cases}$$

Then $M'(t^*) \leq 0$ in the viscosity sense if $\phi'(t^*) \leq 0$, see [4, Definition 2.2] for a definition of viscosity solutions.

From (2.2) and (2.3), we have

$$z_{n^*(t)}(t) \leqslant M(t) \leqslant \phi(t), \quad z_{n^*(t^*)}(t^*) = M(t^*) = \phi(t^*), \tag{2.5}$$

thus $\phi'(t) = \frac{\mathrm{d}}{\mathrm{d}t} z_{n^*(t)}(t)$ at $t = t^*$, since $z_{n^*(t)}, \phi$ are sufficiently smooth ($X,\ Y \in C^1([0,T), \ell^\infty)$).

If $\phi'(t) = \frac{\mathrm{d}}{\mathrm{d}t} z_{n^*(t)}(t) \leq 0$ at $t = t^*$, then we have $M'(t^*) \leq 0$ in the viscosity sense. Thus using the Gronwall inequality (which in the viscosity solutions framework is nothing else but the comparison principle), we deduce

$$M(t) \leq M(0).$$

But $z_n(0) = x_n(0) - y_n(0) \leq 0$ for all $n \in \mathbb{Z}$, thus $M(t) \leq M(0) \leq 0$.

Therefore our goal now is to show that indeed $\frac{\mathrm{d}}{\mathrm{d}t} z_{n^*(t)}(t) \leqslant 0$ at $t = t^*$. Set $n^* = n^*(t^*)$, using the Taylor expansion of the function G, we have

$$\begin{aligned}\frac{\mathrm{d}z_{n^*}(t)}{\mathrm{d}t} &= \frac{\mathrm{d}x_{n^*}(t)}{\mathrm{d}t} - \frac{\mathrm{d}y_{n^*}(t)}{\mathrm{d}t} = G_{n^*}(X(t)) - G_{n^*}(Y(t)) \\ &= \sum_{m \in \mathbb{Z}} \partial_m G_{n^*}(\Theta(t))(x_m(t) - y_m(t)),\end{aligned}$$

where $\Theta(t) = \alpha X(t) + (1-\alpha) Y(t)$ for some $\alpha \in (0,1)$. Here $\partial_m G_n(X)$ is to be understood as

$$\partial_m G_n(X) := \frac{\mathrm{d}G_n(X)}{\mathrm{d}x_m}.$$

In particular for $t = t^*$, we obtain

$$\begin{aligned}\frac{\mathrm{d}z_{n^*}(t^*)}{\mathrm{d}t} &= \partial_{n^*} G_{n^*}(\Theta(t^*)) z_{n^*}(t^*) + \sum_{\substack{m \in \mathbb{Z} \\ m \neq n^*}} \partial_m G_{n^*}(\Theta(t^*))(x_m(t^*) - y_m(t^*)) \\ &\leqslant \partial_{n^*} G_{n^*}(\Theta(t^*)) z_{n^*}(t^*) + z_{n^*}(t^*) \sum_{\substack{m \in \mathbb{Z} \\ m \neq n^*}} \partial_m G_{n^*}(\Theta(t^*)) \\ &= z_{n^*}(t^*) \sum_{m \in \mathbb{Z}} \partial_m G_{n^*}(\Theta(t^*)) = 0.\end{aligned} \tag{2.6}$$

The inequality in the middle line and the last equality in the above computations can be justified as follow.

First, we notice that for every $m \neq n^*$ and by the assumption on monotonicity of the function g, we have

$$\partial_m G_{n^*}(\Theta(t^*)) = g_x(\Theta_m(t) - \Theta_{n^*}(t), m - n^*)\alpha \geqslant 0.$$

Here g_x denotes the partial derivative of $g = g(x,y)$ with respect to the first variable x.

Second, we can calculate explicitly $\partial_{n^*} G_{n^*}(\Theta(t^*))$. Namely, by the structure of the function G, we get

$$\partial_{n^*} G_{n^*}(\Theta(t^*)) = -\sum_{m \neq n^*} g_x(\Theta_m(t) - \Theta_{n^*}(t), m - n^*)\alpha.$$

Summing up all the derivatives of G, we arrive at the last equality of (2.6).

Step 2: $n^*(t^*) = +\infty$.
Then there exists a subsequence n_k such that

$$M(t^*) = \sup_{n\in\mathbb{Z}} z_n(t^*) = \lim_{k\to+\infty} z_{n_k}(t^*). \tag{2.7}$$

Let us redefine the sequences up to shift the indices, we have

$$\left\{\begin{array}{ll} x_n^k(t) = x_{n+n_k}(t) \to & x_n^\infty \\ y_n^k(t) = y_{n+n_k}(t) \to & y_n^\infty \\ z_n^k(t) = z_{n+n_k}(t) \to & z_n^\infty = x_n^\infty - y_n^\infty \end{array}\right| \quad \text{as} \quad k \to +\infty.$$

The convergence of the sequences takes place up to subsequence of k, since x_n^k, y_n^k and z_n^k are bounded.

Moreover, we have from (2.7) that

$$\begin{aligned} M(t^*) = \lim_{k\to+\infty} z_{n_k}(t^*) &= \lim_{k\to+\infty} z_0^k(t^*) \\ &= z_0^\infty(t^*) \le \sup_{n\in\mathbb{Z}} z_n^\infty(t^*) \end{aligned}$$

and

$$\begin{aligned} M(t^*) &= \sup_{n\in\mathbb{Z}} z_n(t^*) \\ &\ge z_{n+n_k}(t^*) = z_n^k(t^*) \quad \text{for all } n \in \mathbb{Z}, \end{aligned}$$

i.e. $M(t^*) \ge z_n^\infty(t^*)$, and hence $M(t^*) \ge \sup_{n\in\mathbb{Z}} z_n^\infty(t^*)$.

Therefore,

$$M(t^*) = z_0^\infty(t^*) = \sup_{n\in\mathbb{Z}} z_n^\infty(t^*),$$

and hence $n^* = 0$. In addition, we have

$$z_n^\infty(0) = x_n^\infty(0) - y_n^\infty(0) \le 0.$$

Thus, applying the result of Step 1 for $z_n^\infty(t)$, we prove the desired result. ∎

3 Existence and uniqueness of solution

We give, in this section, the proof of Theorem (1.2) which combines the classical Cauchy-Lipschitz theorem [2, Thm 7.3, p. 184] and the comparison principle, Lemma 2.1.

Proof of Theorem 1.2. In the proof we argue in several steps.

Step 0: Properties of the function f.
Consider the function f be defined in (1.4a). Clearly, we have $f(\cdot, y) \in C^\infty(\mathbb{R})$ and $f(\pm\infty, y) = \mp 0$ for every $y \in \mathbb{Z}\backslash\{0\}$ fixed. Moreover, $f(\cdot, y)$ is antisymmetric and there exists $x_y = \sqrt{3-\sqrt{2}}|y|$ such that

$$f(x_y, y) = \max_{x\in\mathbb{R}} f(x, y), \quad f(-x_y, y) = \min_{x\in\mathbb{R}} f(x, y)$$

and $f(\cdot, y)$ is non-decreasing over $[-x_y, x_y]$, see for instance Figure 1.

Moreover, we see that for fixed $y \in \mathbb{Z}\backslash\{0\}$

$$\left|\frac{\mathrm{d}}{\mathrm{d}x} f(x, y)\right| \leqslant \frac{\mathrm{d}}{\mathrm{d}x} f(0, y) = \frac{1}{y^2}. \tag{3.1}$$

Hence, f is globally Lipschitz continuous over $\mathbb{R}$ with $\frac{1}{y^2}$ Lipschitz constant depending on fixed y.

Step 1: Existence of a unique global solution for (1.3)*.*
Let $X = (x_i)_{i\in\mathbb{Z}},\ Y = (y_i)_{i\in\mathbb{Z}} \in \ell^\infty$. Using (3.1), we have

$$\begin{aligned}
\|F(X) - F(Y)\|_{\ell^\infty} &= \max_{i\in\mathbb{Z}} |F_i(X) - F_i(Y)| \\
&= \max_{i\in\mathbb{Z}} \Big|\sum_{j\neq i} f(x_j - x_i, j-i) - f(y_j - y_i, j-i)\Big| \\
&\leqslant \max_{i\in\mathbb{Z}} \sum_{j\neq i} |f(x_j - x_i, j-i) - f(y_j - y_i, j-i)| \\
&\leqslant \max_{i\in\mathbb{Z}} \sum_{j\neq i} \frac{1}{(j-i)^2}\Big(|x_j - y_j| + |x_i - y_i|\Big) \\
&\leqslant 4\|X - Y\|_{\ell^\infty} \sum_{k=1}^{+\infty} \frac{1}{k^2}.
\end{aligned}$$

Thus

$$\|F(X) - F(Y)\|_{\ell^\infty} \leq \frac{2}{3}\pi^2 \|X - Y\|_{\ell^\infty}. \tag{3.2}$$

Therefore, using the classical Cauchy-Lipschitz theorem [2, Thm 7.3, p. 184], there exists a unique solution $X \in C^1([0, +\infty), \ell^\infty)$ of (1.3).

Step 2: Invariance: $X(t) \in \Omega$ for every $t \geq 0$.
In this step we show that if $X(0) = X^0 \in \Omega$, then the solution $X(t)$ given in Step 1 satisfies

$$X(t) \in \Omega \quad \text{for every} \quad t \geq 0.$$

Step 2.1: Variant system of (1.3).
For $y \in \mathbb{Z}\backslash\{0\}$ fixed, define a new function $\tilde{f} = \tilde{f}(x, y)$ as follows

$$\begin{cases} \tilde{f}(x,y) = f(x,y) & \text{for } x \in [-x_y, x_y], \\ \tilde{f}(x,y) = f(x_y,y) & \text{for all } x \geqslant x_y, \\ \tilde{f}(x,y) = f(-x_y,y) & \text{for all } x \leqslant -x_y. \end{cases} \tag{3.3}$$

Clearly, $\tilde{f}$ is Lipschitz and non-decreasing with respect to the first variable over the whole space. Moreover, since $\frac{\mathrm{d}}{\mathrm{d}x} f(\pm x_y, y) = 0$ for fixed $y \neq 0$, then $\tilde{f}$ is C^1 with respect to the first variable on $\mathbb{R}$.

Then we consider the following system

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\tilde{X}(t) = \tilde{F}(\tilde{X}(t)) \quad t \geqslant 0, \\ \tilde{X}(0) = X^0 \in \Omega \cap \ell^\infty, \end{cases} \tag{3.4}$$

where again $\tilde{X}(t) = (\tilde{x}_i(t))_{i\in\mathbb{Z}}$ and $\tilde{F}(\tilde{X}) = (\tilde{F}_i(\tilde{X}))_{i\in\mathbb{Z}}$, with

$$\tilde{F}_i(\tilde{X}(t)) := \sum_{j\neq i} \tilde{f}(\tilde{x}_j - \tilde{x}_i, j - i). \tag{3.5}$$

Similarly to Step 1 we show for every $\tilde{X} = (\tilde{x}_i)_{i\in\mathbb{Z}}$, $\tilde{Y} = (\tilde{y}_i)_{i\in\mathbb{Z}}$, that

$$\|\tilde{F}(\tilde{X}) - \tilde{F}(\tilde{Y})\|_{\ell^\infty} \leq \frac{2}{3}\pi^2 \|\tilde{X} - \tilde{Y}\|_{\ell^\infty}.$$

Therefore, using the classical Cauchy-Lipschitz theorem [2, Thm 7.3, p. 184], there exists a unique solution $\tilde{X} \in C^1([0,+\infty), \ell^\infty)$ of the variant problem (3.4).

Step 2.2: $\tilde{X}(t) \in \Omega$ for every $t \geq 0$.
We have $\tilde{X}(0) = X^0 \in \Omega$, i.e.

$$-\sqrt{3 - 2\sqrt{2}}|i - j| \leqslant x_i^0 - x_j^0 \leqslant \sqrt{3 - 2\sqrt{2}}|i - j|, \quad \forall i, j \in \mathbb{Z}.$$

Setting $m = i - j$, we obtain

$$\underline{x}_i^m(0) := x_{i-m}^0 - \sqrt{3 - 2\sqrt{2}}|m| \leqslant x_i^0 \leqslant x_{i-m}^0 + \sqrt{3 - 2\sqrt{2}}|m| =: \overline{x}_i^m(0),$$

for every $i, m \in \mathbb{Z}$.

Moreover, from the definition of the function $\tilde{F}$, see (3.5), it is clear that the problem (3.4) is invariant by translations. Hence,

$$\underline{X}^m = \left(\tilde{x}_{i-m}(t) - \sqrt{3 - 2\sqrt{2}}|m| =: \underline{x}_i^m\right)_{i\in\mathbb{Z}}$$

and

$$\overline{X}^m = \left(\tilde{x}_{i-m}(t) + \sqrt{3-2\sqrt{2}}|m| =: \overline{x}_i^m \right)_{i\in\mathbb{Z}}$$

are two solutions of (3.4) for each $m \in \mathbb{Z}$. Now, since $\tilde{f}$ is non-decreasing, we can apply the comparison principle, Lemma 2.1 (with $T = +\infty$), and deduce that for every $i, m \in \mathbb{Z}$

$$\underline{x}_i^m(t) \leqslant \tilde{x}_i(t) \leqslant \overline{x}_i^m(t) \quad \text{for } t > 0.$$

Hence, $\tilde{X}(t) \in \Omega$ for all $t > 0$.

Step 2.3: $\tilde{X}$ solves (1.3).
We have that $\tilde{X}(t) \in \Omega$ for all $t > 0$. Thus

$$-x_y = -\sqrt{3-2\sqrt{2}}|i-j| \leqslant \tilde{x}_i - \tilde{x}_j \leqslant \sqrt{3-2\sqrt{2}}|i-j| = x_y, \quad \forall i, j \in \mathbb{Z}.$$

However, $\tilde{f}(\cdot, i-j)_{|_{[-x_y, x_y]}} = f(\cdot, i-j)_{|_{[-x_y, x_y]}}$, hence

$$\tilde{F}(\tilde{X}(t)) = F(\tilde{X}(t)) \quad \text{over} \quad t > 0.$$

Therefore, $\tilde{X}$ solves (1.3).

Step 2.4: Conclusion: $X(t) \in \Omega$ for every $t \geq 0$.
Since

$$\tilde{X}(0) = X^0 = X(0),$$

then by the uniqueness of the solution of system (1.3) (See Step 1), we get

$$X(t) = \tilde{X}(t) \in \Omega \quad \text{for every} \quad t \geq 0.$$

Thereupon, we have proved that $X(t)$ is the unique global solution of the problem (1.3)-(1.4).

Step 3: X is periodic.
Assume that $X(0) = X^0$ is N-periodic; i.e. $x_i^0 = x_{i+N}^0$ for every $i \in \mathbb{Z}$. Define $Y = (y_i)_{i\in\mathbb{Z}} = (x_{i+N})_{i\in\mathbb{Z}}$, where we recall that $X = (x_i)_{i\in\mathbb{Z}}$. Then X and Y are two solutions of (1.3) with $X(t)$,$Y(t) \in \Omega$ for all $t \geq 0$. Moreover, we have $Y(0) = (x_{i+N}^0)_{i\in\mathbb{Z}} = X^0$ ($Y(0) \leq X^0$ and $X^0 \leq Y(0)$). Since f is non-decreasing over Ω, then using the comparison principle (Lemma 2.1 with $T = +\infty$), we deduce that

$$Y(t) = X(t) \quad \text{for every } t \geq 0,$$

i.e $x_i = x_{i+N}$ for every $t \geq 0$. ■

4 Convergence to flat walls

The aim of this section is to prove that under the periodicity assumption imposed on the initial data, the solution constructed in Theorem 1.2 converges to a special stationary solution of the problem (1.3). Precisely, in this section, we prove Theorem 1.3.

Proof of Theorem 1.3.

Step 0: preliminary (reformulation of (1.3)*).*
Let $X = (x_i)_{i\in\mathbb{Z}} \in C^1([0,\infty), \Omega \cap \ell^\infty)$ be a N-periodic (*i.e.* $x_{i+N} = x_i$) solution of (1.3). For $i = 1, ..., N$ we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}x_i(t) &= \sum_{j\neq i} f(x_j - x_i, j-i)\\ &= \sum_{\substack{j=1\\ j\neq i}}^{N} \sum_{k\in\mathbb{Z}} f(x_{j+kN} - x_i, j-i+kN).\end{aligned}$$

Using the periodicity of X ($x_{j+kN} = x_j$), we get that

$$\frac{\mathrm{d}}{\mathrm{d}t}x_i(t) = \sum_{\substack{j=1\\ j\neq i}}^{N} \sum_{k\in\mathbb{Z}} f(x_j - x_i, j-i+kN).$$

Hence, we can transform (1.1) into the following equation

$$\frac{\mathrm{d}}{\mathrm{d}t}x_i(t) = \sum_{\substack{j=1\\ j\neq i}}^{N} g(x_j - x_i, j-i), \quad i = 1, \ldots, N, \tag{4.1}$$

where $g(x,y) = \sum\limits_{k\in\mathbb{Z}} f(x, y+kN)$. Moreover, since for every $y \neq 0$, the map $x \mapsto f(x,y)$ is Lipschitz with $\frac{1}{y^2}$ Lipschitz constant (see Step 0, in the proof of Theorem 1.2), $g(0,y) = f(0,y) = 0$ and $x \in \ell^\infty$, then

$$|g(x,y)| = \left|\sum_{k\in\mathbb{Z}} f(x, y+kN) - f(0, y+kN)\right| \le \sum_{k\in\mathbb{Z}} \frac{1}{(y+kN)^2}|x| \le \mathcal{M} \tag{4.2}$$

for some $\mathcal{M} > 0$. Hence, g is uniformly bounded in x.

In order to prove the convergence of the solution, we set

$$M(t) = \frac{1}{2}\sum_{i=1}^{N} x_i^2(t) \tag{4.3}$$

and we argue by steps.

Step 1: M is non-increasing.
Indeed, we have

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1}^{N} x_i^2(t) = \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} x_i(t)\, g(x_j(t)-x_i(t), j-i)$$

$$= \sum_{i=1}^{N}\sum_{j=i+1}^{N} x_i(t)\, g(x_j(t)-x_i(t), j-i) + \sum_{i=1}^{N}\sum_{j=1}^{i-1} x_i(t)\, g(x_j(t)-x_i(t), j-i)$$

$$= \sum_{i=1}^{N}\sum_{k=1}^{N-i} x_i(t)\, g(x_{i+k}(t)-x_i(t), k) - \sum_{j=1}^{N}\sum_{i=j+1}^{N} x_i(t)\, g(x_i(t)-x_j(t), i-j)$$

$$= \sum_{i=1}^{N}\sum_{k=1}^{N-i} x_i(t)\, g(x_{i+k}(t)-x_i(t), k) - \sum_{j=1}^{N}\sum_{k=1}^{N-j} x_{j+k}(t)\, g(x_{j+k}(t)-x_j(t), k)$$

$$= \sum_{i=1}^{N}\sum_{k=1}^{N-i} (x_i(t)-x_{i+k}(t))\, g(x_{i+k}(t)-x_i(t), k) \leqslant 0.$$

First, let us mention that due to the fact that the function $f = f(x,y)$, defined by (1.4a) is symmetric in y and antisymmetric in x, the function $g = g(x,y)$ possesses such property as well. Moreover, as a result of the boundedness of the function $g(\cdot,y)$ (which comes form the Lipschitz condition of $f(\cdot,y)$) and the fact that only finite sums are considered, we are allowed to use Fubini's theorem and change the order of summation. These facts justify the third equality.

The inequality is obtained by the fact that each single expression under the sums is nonpositive due to the definitions of the functions g, f and the fact that $X(t) \in \Omega \cap \ell^\infty$ for $t \geqslant 0$ (see Remark 1.1).

Finally, we conclude that $M(t) \to M_0$ as $t \to \infty$ since $M(t)$ is nonnegative and non-increasing.

Step 2: limit of $X(t)$ as $t \to +\infty$.
Let us define $X^n(t) := X(t+n)$. Then X^n is a solution of (1.3). Since $f(x,y)$ is Lipschitz with $\frac{1}{y^2}$ Lipschitz constant (independent if x), hence $\frac{\mathrm{d}}{\mathrm{d}t}X^n(t) \in \ell^\infty$ uniformly in n. Using Ascoli's theorem, up to some subsequence, $X^n(t) \to X^\infty(t)$ as $n \to \infty$ for every $t > 0$. Thus, we can write

$$M_0 = \lim_{n\to\infty} M(t+n) = \lim_{n\to\infty} \frac{1}{2}\sum_{i=1}^{N}\left(x_i^n(t)\right)^2 = \frac{1}{2}\sum_{i=1}^{N}\left(x_i^\infty(t)\right)^2. \tag{4.4}$$

Since X^n is a solution of (4.1) and $X^n(t) \in \Omega \cap \ell^\infty$, then the limit X^∞ is a classical solution and $X^\infty(t) \in \Omega \cap \ell^\infty$. Therefore, repeating all the computations performed in Step 1 for X^∞, we arrive at

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}t} M_0 &= \frac{\mathrm{d}}{\mathrm{d}t} \frac{1}{2} \sum_{i=1}^{N} \left(x_i^\infty(t)\right)^2 \\ &= \sum_{i=1}^{N} \sum_{k=1}^{N-i} (x_i^\infty(t) - x_{i+k}^\infty(t))\, g(x_{i+k}^\infty(t) - x_i^\infty(t), k). \end{aligned}$$

Since the solution lives in Ω, $g(x_{i+k}^\infty(t) - x_i^\infty(t), k)$ and $x_{i+k}^\infty(t) - x_i^\infty(t)$ have the same sign (see Remark 1.1), then

$$(x_i^\infty(t) - x_{i+k}^\infty(t))\, g(x_{i+k}^\infty(t) - x_i^\infty(t), k) \leq 0$$

for all $i \in \{1, .., N-1\}$ and $k \in \{1, ..., N-i\}$. Thus, either

$$x_i^\infty(t) = x_j^\infty(t) \quad \text{for all} \quad i = 1, \dots, N-1 \text{ and } j = i+1, \dots, N, \tag{4.5}$$

or we have $g = 0$. However, since $X^\infty(t) \in \Omega \cap \ell^\infty$, then $g = 0$ immediately implies (4.5) (see (1.4a) and the definition of g).

Therefore, we get from (4.5) that

$$x_1^\infty(t) = x_2^\infty(t) = \dots = x_N^\infty(t).$$

Next, we plug X^∞ into the equation (4.1) to see that indeed $\frac{\mathrm{d}}{\mathrm{d}t} x_i^\infty(t) = 0$ (since $g(0, y) = 0$); thus, $x_i^\infty(t) = x_i^\infty(0) = c$, for all $i = 1, \dots, N$, and for some $c \in \mathbb{R}$. Moreover, we can write the explicit value of M_0, i.e.

$$M_0 = \frac{1}{2} N c^2.$$

Now take another convergent subsequence, $X^m(t)$ of $X(t)$ such that $X^m(t) \to \overline{X}^\infty(t)$ as $m \to \infty$. Repeating all the calculations performed for the sequence X^n, we may show that $\overline{x}_i^\infty(t) = \overline{x}_i^\infty(0) = b$ for all $i = 1, \dots, N$, $t \geqslant 0$ and some $b \in \mathbb{R}$. As before we conclude that

$$M_0 = \frac{1}{2} N b^2.$$

Thus, $b = c$, because we may assume, without loss of generality, that $b, c \geqslant 0$, since the problem (4.1) is invariant by translations and the initial data can be shifted to be positive.

This implies that the accumulation point of X is unique. Hence, $x_i(t) \to c$ as $t \to \infty$ for all $i = 1, \dots, N$.

Step 3: identification of the limit.
In this step we prove that the barycenter is preserved in time, i.e.

$$\sum_{i=1}^{N} x_i(t) = \sum_{i=1}^{N} x_i(0) \quad \text{for all} \quad t > 0,$$

which allows us to determine the value of the constant c.

We have

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=1}^{N} x_i(t) = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_j - x_i, j - i).$$

But

$$\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_j - x_i, j - i) = \sum_{j=1}^{N} \sum_{\substack{i=1 \\ i\neq j}}^{N} g(x_j - x_i, j - i) = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_i - x_j, i - j),$$

where we have changed the order of summation in the first equality (this is possible because g is a bounded function), and we replaced i and j in the second equality. Moreover, since $g(x, y)$ is antisymmetric w.r.t. x and symmetric w.r.t. y (because f antisymmetric and symmetric w.r.t. x and y respectively), then we get

$$\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_j - x_i, j - i) = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_i - x_j, i - j) = -\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_j - x_i, j - i).$$

Therefore, we deduce that

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=1}^{N} x_i(t) = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} g(x_j - x_i, j - i) = 0,$$

and hence

$$\sum_{i=1}^{N} x_i(t) = \sum_{i=1}^{N} x_i(0).$$

Finally, since $x(t) \to c$ as $t \to \infty$, we conclude that

$$\sum_{i=1}^{N} x_i(0) = \lim_{t\to\infty} \sum_{i=1}^{N} x_i(t) = Nc,$$

i.e.

$$c = \frac{1}{N} \sum_{i=1}^{N} x_i(0) \tag{4.6}$$

thus, we have proved the desired result. $\blacksquare$.

5 From micro to macro model

We show in this section the ℓ^P contraction estimate of periodic solutions of (1.3)-(1.4), namely we give the proof of Proposition 1.4.

Proof of Proposition 1.4. Let $X = (x_i)_{i\in\mathbb{Z}}$ and $Y = (y_i)_{i\in\mathbb{Z}}$ be a N-periodic (*i.e.* $x_{i+N} = x_i$, $y_{i+N} = y_i$) solution of (1.3) of the class $C^1([0,\infty), \Omega \cap \ell^\infty)$. We proceed as in Section 4, Step 1. First, without loss of generality, we may transform (1.1) into the following equation

$$\frac{\mathrm{d}}{\mathrm{d}t} x_i(t) = \sum_{\substack{j=1\\ j\neq i}}^{N} g(x_j - x_i, j-i), \quad i = 1, \ldots, N,$$

with the function $g(x,y) = \sum\limits_{k\in\mathbb{Z}} f(x, y+kN)$ uniformly bounded in x. Thus, we calculate

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{p}\big\|X(t)-Y(t)\big\|_p^p = \sum_{i=1}^{N}\big|x_i(t)-y_i(t)\big|^{p-2}\big(x_i(t)-y_i(t)\big)\big(\dot{x}_i(t)-\dot{y}_i(t)\big) = \\
&\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\big|x_i(t)-y_i(t)\big|^{p-2}\big(x_i(t)-y_i(t)\big)\big(g(x_j(t)-x_i(t), j-i)-g(y_j(t)-y_i(t), j-i)\big) \\
&= \sum_{i=1}^{N}\sum_{k=1}^{N-i}\underbrace{\Big(\big|x_i(t)-y_i(t)\big|^{p-2}\big(x_i(t)-y_i(t)\big)-\big|x_{i+k}(t)-y_{i+k}(t)\big|^{p-2}\big(x_{i+k}(t)-y_{i+k}(t)\big)\Big)}_{\mathcal{I}_1} \\
&\qquad\cdot\underbrace{\Big(g(x_{i+k}(t)-x_i(t), k)-g(y_{i+k}(t)-y_i(t), k)\Big)}_{\mathcal{I}_2} \leqslant 0.
\end{aligned}$$

Let us mention here that due to the fact that the function $f = f(x,y)$, defined by (1.4a), is symmetric in y and antisymmetric in x, the function $g = g(x,y)$ possesses such property as well. Moreover, as a result of the boundedness of the function $g(\cdot, y)$ (which comes form the Lipschitz condition of $f(\cdot, y)$) and the fact that only finite sums are considered, we are allowed to use Fubini's theorem and change the order of summation. These facts justify the third equality.

Furthermore, we notice that for fixed $y \in \mathbb{Z}$ the function $f(x,y)$ is nondecreasing in the variable x provided $|x| \leqslant \sqrt{3-2\sqrt{2}}|y|$. Hence, by definition the function $g(x,y)$ is also nondecreasing in the variable x under the same condition on x. Suppose now that $\mathcal{I}_2 \leqslant 0$. This immediately implies, in view of the above information, that $x_{i+k}(t) - y_{i+k}(t) \leqslant x_i(t) - y_i(t)$; hence, $\mathcal{I}_1 \geqslant 0$. On the contrary, if $\mathcal{I}_2 \geqslant 0$, then $\mathcal{I}_1 \leqslant 0$. Hence, we conclude

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{p}\|X(t) - Y(t)\|_p^p \leqslant 0,$$

which completes the proof. ■

Corollary 5.1 (l^p contraction for a rescaling of x_i)**.** *Let $p \geqslant 2$. Fix $\varepsilon > 0$ and let us define new variables in the following way*

$$x_i(t) = \frac{1}{\varepsilon}u^\varepsilon(\varepsilon i, \varepsilon t), \quad \forall i \in \mathbb{Z}.$$

Then the above theorem reads as

$$\|u^\varepsilon(\cdot, \tau) - v^\varepsilon(\cdot, \tau)\|_p \leqslant \|u_0^\varepsilon - v_0^\varepsilon\|_p.$$

6 Numerical experiments

Here we present results of some numerical experiments to confirm the results obtained in Theorem 1.3. We construct an adaptive scheme as follows. Let $N > 0$ denote the total number of interacting particles. Let Δt denote a time-step and let us define an approximate solution of (1.3) by a solution $X^n = (X_1^n, \ldots, X_N^n)$ of the following forward Euler scheme

$$X^{n+1} = X^n + \Delta t F(X^n) \stackrel{def}{=} S(X^n). \tag{6.1}$$

Lemma 6.1 (Monotonicity of the scheme)**.** *The scheme derived in* (6.1) *is monotone if and only if the time-step satisfies $\Delta t \leqslant \frac{3}{\pi^2}$ and the initial data $X^0 \in \Omega$ defined in* (1.5)*.*

Proof. To prove the monotonicity it is enough to show that $\partial_j S_i(X^n) \geqslant 0$ for all $i, j = 1, \ldots, N$. First, we notice that due to Lemma 2.1 we get $X^n \in \Omega$ for all $n \in \mathbb{N}$.

Step 1: $j \neq i$.

$$\partial_j F_i(X^n) = \Delta t\, f_x(X_j^n - X_i^n, j - i) \geqslant 0, \tag{6.2}$$

since considered function f is nondecreasing with respect to the first variable.

Step 2: $j = i$.

$$\begin{aligned}
\partial_i F_i(X^n) &= 1 - \Delta t \sum_{\substack{j=1 \\ j \neq i}}^{N} f_x(X_j^n - X_i^n, j - i) \\
&\geqslant 1 - \Delta t \sum_{\substack{j=1 \\ j \neq i}}^{N} f_x(0, j - i) \\
&\geqslant 1 - \Delta t \sum_{\substack{j \in \mathbb{Z} \\ j \neq i}} \frac{1}{(j-i)^2} \\
&\geqslant 1 - \Delta t \frac{\pi^2}{3} \geqslant 0.
\end{aligned}$$

To justify the first inequality we use the properties of the function f described in the proof of Theorem 1.2 Step 1. Moreover, we extend the finite sum by its infinite version and we conclude its nonnegativity. ■

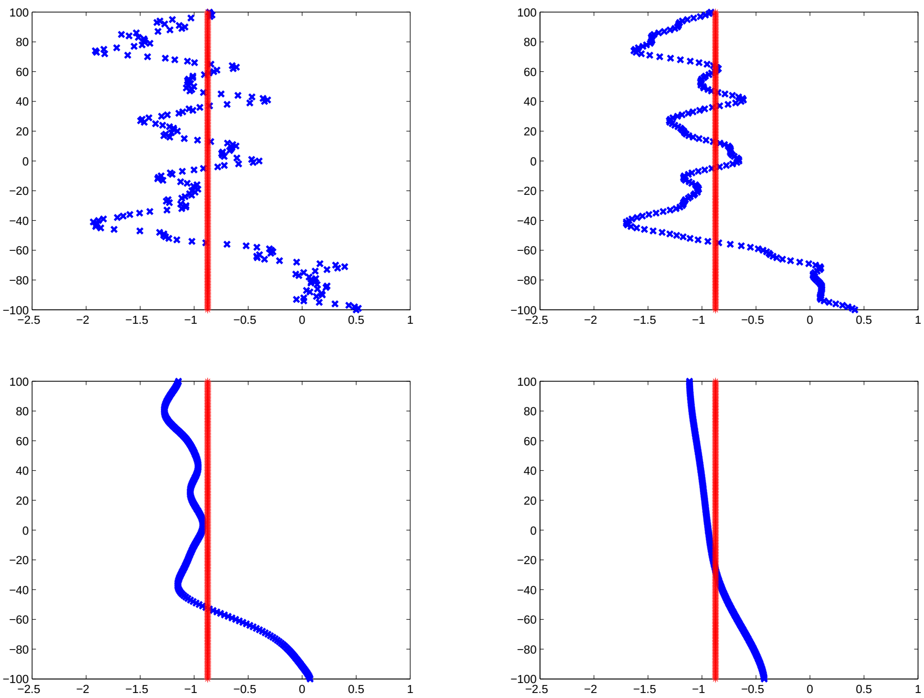

Figure 3: Evolution of dislocations of (1.3) with initial data $X^0 \in \Omega$.

In our numerical experiments we assume the initial data $X^0 \in \Omega \cap \ell^\infty$ which is denoted by "x" on the left-upper plot in Figure 3. Furthermore, in every picture, by "*" we emphasised what the limit solution (by Theorem 1.3 the limit solution is at the barycenter of initial data) is. In Figure 3 we observe the evolution of dislocations which eventually converge.

However, we may also consider the initial data $X^0 \in \overline{\Omega}$ where

$$\overline{\Omega} = \left\{ X : \sqrt{3 - 2\sqrt{2}}\, |i-j| < |x_i - x_j| < |i-j| \right\}, \tag{6.3}$$

see the blue region in Figure 2. It is worth noticing that for such initial data, the force acting on dislocations is still attractive; however, we do not have a comparison principle and we cannot guarantee that solution stays in $\overline{\Omega}$, but we can perform numerical experiments to see what happen with dislocations.

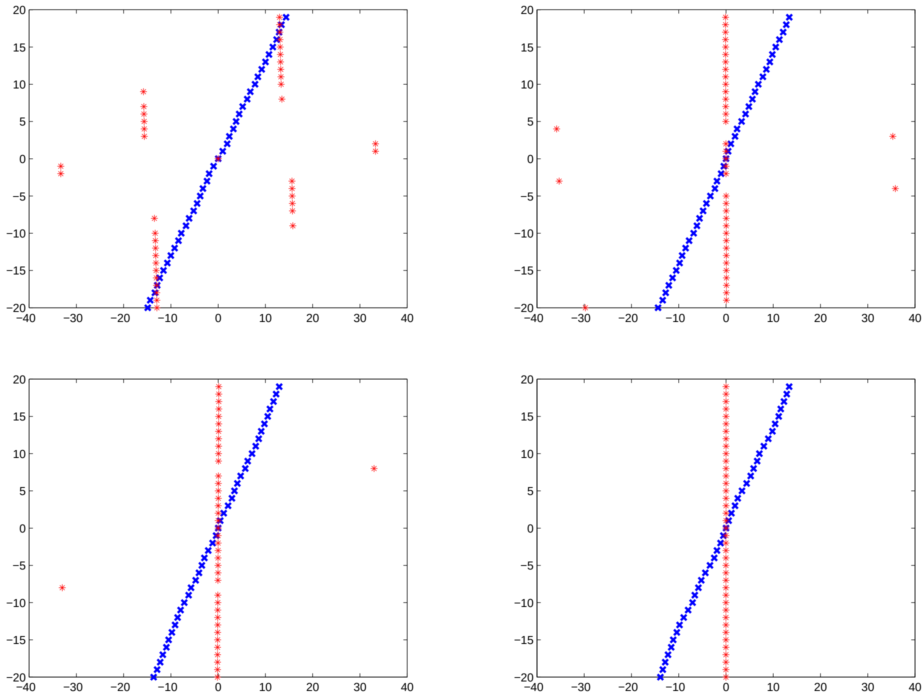

Figure 4: Evolution of dislocations of (1.3) with initial data $X^0 \in \overline{\Omega}$. Each simulation starts with different initial data.

In the above pictures we can see that even small perturbation of initial data produces completely different solutions. The only one (right-lower plot in Figure 4) converged to a flat wall, while the remainder does not.

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